Towards Uncertainty Quantification in 21st Century Sea-Level Rise Predictions: PDE Constrained Optimization as a First Step in Bayesian Calibration and Forward Propagation

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CCR Center for Computing Research

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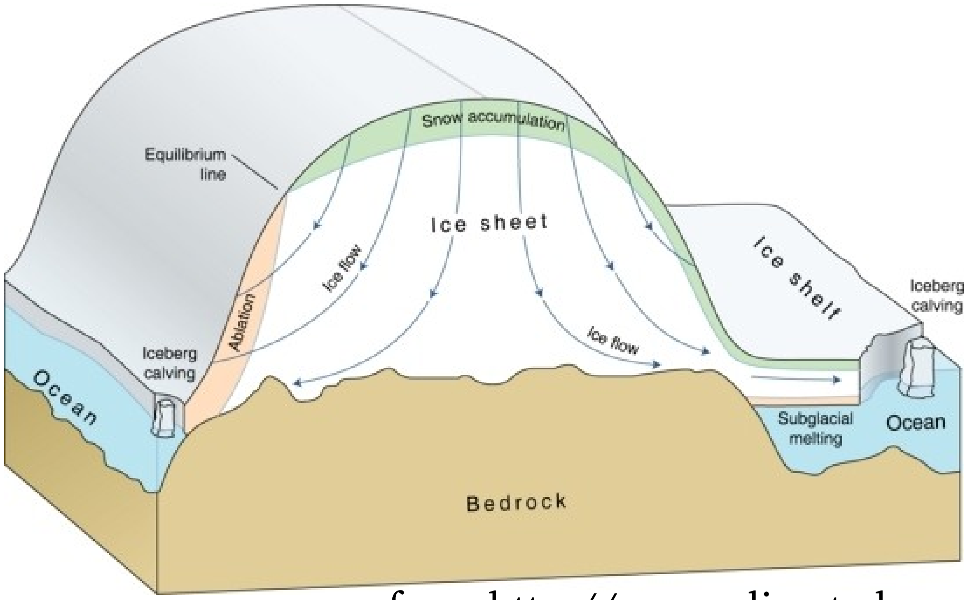
Brief introduction and motivation

- Modeling ice sheets (Greenland and Antarctica) dynamics is essential to provide estimates for sea level rise in next decades to centuries.

- Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) and can be modeled with nonlinear Stokes equation.

- Greenland and Antarctica ice sheets store most of the fresh water on hearth.
  They have a shallow geometry (thickness up to 3km, horizontal extensions of thousands of km).



from http://www.climate.be

Problem definition

Our Quantity of Interest (QoI) in ice sheet modeling:

total ice mass loss/gain by, e.g., 2100 → **sea level rise prediction**

Main sources of uncertainty:

- climate forcings (e.g. ***Surface Mass Balance -SMB***)
- **basal friction**
- **bedrock topography (thickness)**
- geothermal heat flux
- model parameters (e.g. Glen's Flow Law exponent)

Problem definition

Ultimate goal:
quantify the QoI and related uncertainties

Work flow:

- Perform *adjoint-based deterministic inversion* to estimate initial ice sheet state (i.e. characterize the present state of ice sheet to be used for performing prediction runs).
- Use deterministic inversion to characterize the parameter distribution (i.e, use the inverted field as mean field of the parameter distribution and approximate its covariance using sensitivities/Hessian).
- Perform *Bayesian Calibration* (see next talk by Irina Tezaur).
- Perform *Forward Propagation* (see next talk by Irina Tezaur).

Ice Sheet Modeling

Ice momentum equations

- **Ice flow equations** (momentum and mass balance)

$$\begin{cases} -\nabla \cdot \sigma = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

with:

$$\sigma = 2\mu \mathbf{D} - pI, \qquad \mathbf{D}_{ij}(\mathbf{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Nonlinear viscosity:

$$\mu = \frac{1}{2}\alpha(T)\,|\mathbf{D}(\mathbf{u})|^{\frac{1}{n}-1}, \quad n \geq 1, \quad (\text{tipically } n \simeq 3)$$

Viscosity is singular when ice is not deforming

Stokes approximations in different regimes

$\text{Stokes}(\mathbf{u}, p)$

$$\begin{cases} -\nabla \cdot (2\mu \mathbf{D}(\mathbf{u}) - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

$\downarrow$

$\text{FO}(u, v)$

First Order* or
Blatter-Pattyn model

$$-\nabla \cdot \left(2\mu \tilde{\mathbf{D}} - \rho g (s - z)\mathbf{I}\right) = \mathbf{0}$$

Dukowicz, Price and Lipscomb, 2010. J. Glaciol

Stokes approximations in different regimes

$$\text{Stokes}(\mathbf{u}, p)$$

$$\begin{cases} -\nabla \cdot (2\mu \mathbf{D}(\mathbf{u}) - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

Drop terms using **scaling argument** based on the fact that ice sheets are shallow

$$\mathbf{D}(\mathbf{u}) = \begin{bmatrix} u_x & \frac{1}{2}(u_y + v_x) & \frac{1}{2}(u_z + \cancel{w_x}) \\ \frac{1}{2}(u_y + v_x) & v_y & \frac{1}{2}(v_z + \cancel{w_y}) \\ \frac{1}{2}(u_z + \cancel{w_x}) & \frac{1}{2}(v_z + \cancel{w_y}) & w_z \end{bmatrix} \qquad \mathrm{u} := \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

$$\mu = \mu(|\mathbf{D}(\mathbf{u})|)$$

$$\text{FO}(u, v)$$

First Order* or Blatter-Pattyn model

*Dukowicz, Price and Lipscomb, 2010. J. Glaciol

Stokes approximations in different regimes

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$$\mu = \mu(|\mathbf{D}(\mathbf{u})|)$$

Quasi-hydrostatic approximation

3rd momentum equation

$$-\cancel{\partial_x(\mu\, u_z)} - \cancel{\partial_y(\mu\, v_z)} - \partial_z(2\mu\, w_z - p) = -\rho g,$$

continuity equation

$$w_z = -(u_x + v_y)$$

$$\Longrightarrow \; p = \rho g(s - z) - 2\mu(u_x + v_y)$$

$$\mathrm{FO}(u, v)$$

First Order* or Blatter-Pattyn model

*Dukowicz, Price and Lipscomb, 2010. J. Glaciol

Stokes approximations in different regimes

$$\text{Stokes}(\mathbf{u}, p)$$

$$\begin{cases} -\nabla \cdot (2\mu \mathbf{D}(\mathbf{u}) - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

Drop terms using **scaling argument** based on the fact that ice sheets are shallow

$$\mathbf{D}(u,v) = \begin{bmatrix} u_x & \frac{1}{2}(u_y + v_x) & \frac{1}{2}(u_z + \cancel{w_x}) \\ \frac{1}{2}(u_y + v_x) & v_y & \frac{1}{2}(v_z + \cancel{w_y}) \\ \frac{1}{2}(u_z + \cancel{w_x}) & \frac{1}{2}(v_z + \cancel{w_y}) & -(u_x + v_y) \end{bmatrix} \qquad \mathrm{u} := \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

$$\mu = \mu(|\mathbf{D}(u,v)|)$$

Quasi-hydrostatic approximation

3rd momentum equation

$$-\cancel{\partial_x(\mu u_z)} - \cancel{\partial_y(\mu v_z)} - \partial_z(2\mu w_z - p) = -\rho g,$$

continuity equation

$$w_z = -(u_x + v_y)$$

$$\Longrightarrow p = \rho g(s - z) - 2\mu(u_x + v_y)$$

$$\mathrm{FO}(u,v)$$

First Order* or Blatter-Pattyn model

$$-\nabla \cdot \left(2\mu \tilde{\mathbf{D}} - \rho g(s - z)\mathbf{I}\right) = \mathbf{0}$$

with $\tilde{\mathbf{D}}(u,v) = \begin{bmatrix} 2u_x + v_y & \frac{1}{2}(u_y + v_x) & \frac{1}{2}u_z \\ \frac{1}{2}(u_y + v_x) & u_x + 2v_y & \frac{1}{2}v_z \end{bmatrix}$

*Dukowicz, Price and Lipscomb, 2010. J. Glaciol

Estimation of ice sheet initial state

Steady state equations and basal sliding conditions

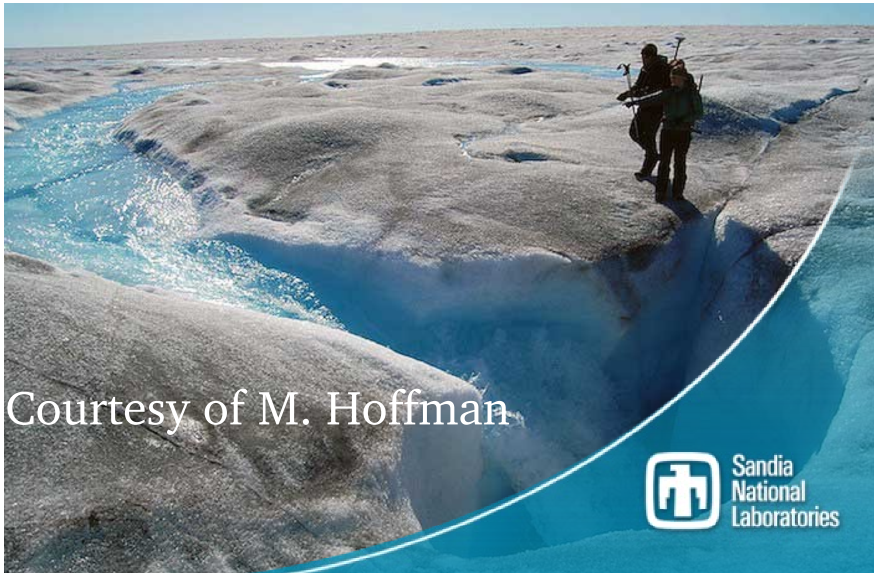
How to prescribe ice sheet mechanical equilibrium:

$$\frac{\partial H}{\partial t} = -\overset{\textit{flux divergence}}{\overset{\downarrow}{\mathrm{div}\,(\mathbf{U}H)}} + \underset{\textit{Surface Mass Balance}}{\underset{\uparrow}{\tau_{\mathrm{smb}}}}, \qquad \mathbf{U} = \frac{1}{H}\int_z \mathbf{u}\,dz.$$

$$\boxed{\mathrm{div}\,(\mathbf{U}H) = \tau_{\mathrm{smb}} - \left\{\frac{\partial H}{\partial t}\right\}^{\mathrm{obs}}}$$

Boundary condition at ice-bedrock interface :

$$(\sigma\mathbf{n} + \beta\mathbf{u})_{||} = \mathbf{0} \quad \text{on} \quad \Gamma_\beta$$



Deterministic Inversion

GOAL

1. Find ice sheet initial state that

- matches observations (e.g. surface velocity, temperature, etc.)
- matches present-day geometry (elevation, thickness)
- is in "equilibrium" with climate forcings (SMB)

by inverting for unknown/uncertain ice sheet model parameters.

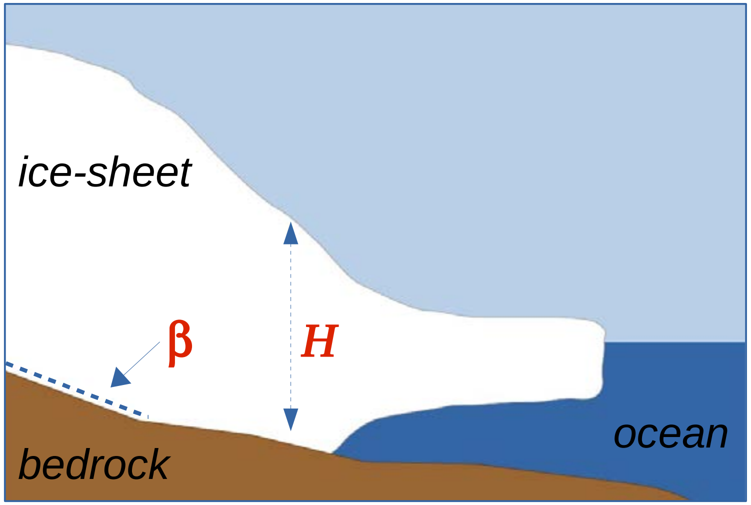
2. Significantly reduce non physical transients without spin-up

Bibliography

- *Arthern, Gudmundsson*, J. Glaciology, 2010
- *Price, Payne, Howat and Smith*, PNAS, 2011
- *Petra, Zhu, Stadler, Hughes, Ghattas*, J. Glaciology, 2012
- *Pollard DeConto*, TCD, 2012
- W. J. J.Van Pelt et al., The Cryosphere, 2013
- *Morlighem et al.* Geophysical Research Letters, 2013
- *Goldberg and Heimbach*, The Cryosphere, 2013
- *Michel et al.*, Computers & Geosciences, 2014
- *Perego, Price, Stadler,* Journal of Geophysical Research, 2014
- *Goldberg et al.,* The Cryosphere Discussions, 2015

Deterministic Inversion

Problem details



Available data/measurements

- *ice extension and surface topography*
- ***surface velocity***
- ***Surface Mass Balance (SMB)***
- ***ice thickness H (sparse measurements)***

Fields to be estimated

- ***ice thickness H (allowed to vary but weighted by observational uncertainties)***
- ***basal friction β (spatially variable proxy for all basal processes)***

Modeling Assumptions

- *ice flow described by* ***nonlinear Stokes equation***
- *ice close to* ***mechanical equilibrium***

Additional Assumption (for now)

- *given* ***temperature field***

Deterministic Inversion

PDE-constrained optimization problem: cost functional

Problem: find initial conditions such that the ice is close to thermo-mechanical equilibrium, given the geometry and the SMB, and matches available observations.

Optimization problem:

find β and H that minimize the functional* $\mathcal{J}$

$$
\begin{aligned}
\mathcal{J}(\beta, H) &= \int_\Sigma \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2 \, ds && \text{surface velocity mismatch} \\
&+ \int_\Sigma \frac{1}{\sigma_\tau^2} \left| \operatorname{div}(\boldsymbol{U} H) - \tau_{\text{smb}} + \left\{ \frac{\partial H}{\partial t} \right\}^{\text{obs}} \right|^2 ds && \text{SMB mismatch} \\
&+ \int_\Sigma \frac{1}{\sigma_H^2} |H - H^{obs}|^2 \, ds && \text{thickness mismatch} \\
&+ \mathcal{R}(\beta, H) && \text{regularization terms.}
\end{aligned}
$$

subject to ice sheet model equations (FO or Stokes)

$\boldsymbol{U}$: computed depth averaged velocity
H: ice thickness
β: basal sliding friction coefficient
τ_s: SMB
$\mathcal{R}(\beta)$ regularization term

*_Perego, Price, Stadler,_ Journal of Geophysical Research, 2014

Inverse Problem

Estimation of ice-sheet initial state

PDE-constraint optimization problem: gradient computation

$$\begin{aligned} \text{Find } (\beta, H) \text{ that minimize} \quad & \mathcal{J}(\beta, H, \mathbf{u}) \\ \text{subject to} \quad & \mathcal{F}(\mathbf{u}, \beta, H) = 0 \quad \leftarrow \quad \text{flow model} \end{aligned}$$

How to compute **total derivatives** of the functional w.r.t. the parameters?

Solve State System: $\mathcal{F}(\mathbf{u}, \beta, H) = 0$

Solve Adjoint System: $\langle \mathcal{F}^*_{\mathbf{u}}(\boldsymbol{\lambda}), \, \boldsymbol{\delta}_{\mathbf{u}} \rangle = \mathcal{J}_{\mathbf{u}}(\boldsymbol{\delta}), \quad \forall \boldsymbol{\delta}_{\mathbf{u}}$

Total derivatives: $\mathcal{G}(\delta_\beta, \delta_H) = \mathcal{J}_{(\beta,H)}(\delta_\beta, \delta_H) - \langle \boldsymbol{\lambda}, \mathcal{F}_{(\beta,H)}(\delta_\beta, \delta_H) \rangle$

Derivative w.r.t. β: $\mathcal{G}_1(\delta_\beta) = \alpha_\beta \int_\Sigma \nabla\beta \cdot \nabla\delta_\beta \, ds - \int_\Sigma \delta_\beta \, \mathbf{u} \cdot \boldsymbol{\lambda} \, ds$

Estimation of ice sheet initial state

Algorithm and Software tools used

ALGORITHM	SOFTWARE TOOLS
Linear Finite Elements on hexahedra	Albany
Quasi-Newton optimization (L-BFGS)	ROL
Nonlinear solver (Newton method)	NOX
Krylov linear solvers/Prec	AztecOO/ML

Trilinos

Albany: C++ finite element library built on Trilinos to enable multiple capabilities:

- Jacobian/adjoints assembled using automatic differentiation (SACADO).
- nonlinear and parameter continuation solvers (NOX/LOCA)
- large scale PDE constrained optimization (Piro/ROL)
- Uncertainty Quantification (using Dakota)
- linear solver and preconditioners (Belos/AztecOO, ML/MeuLu/Ifpack)

Albany

Optimization algorithm:

Reduce Gradient optimization, using L-BFGS.
Storage: 200, Linesearch: backtrack

ROL

Tuminaro, Perego, Tezaur, Salinger, Price, SISC, submitted.
Tezaur, Perego, Salinger, Tuminaro, Price, Hoffman, GMD, 2015
Perego, Price, Stadler, JGR, 2014

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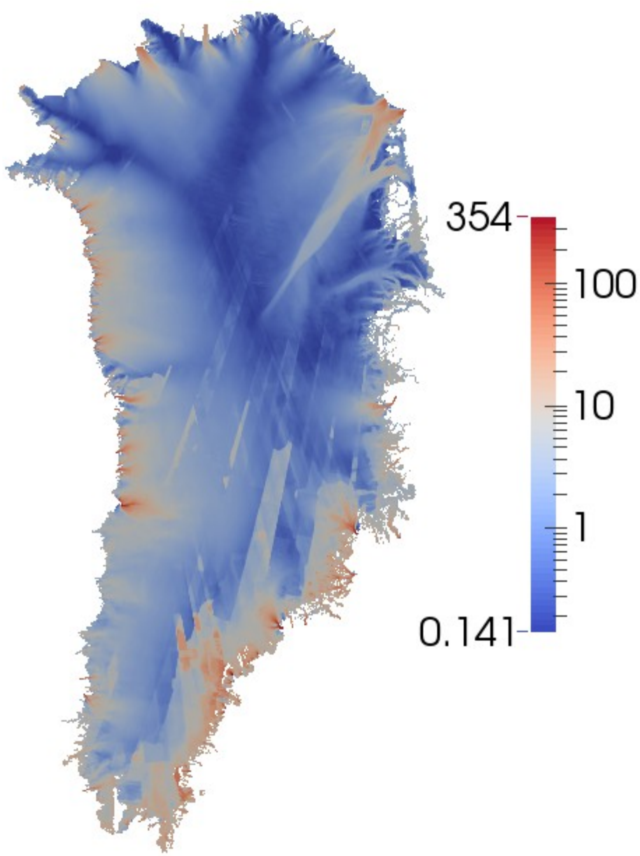
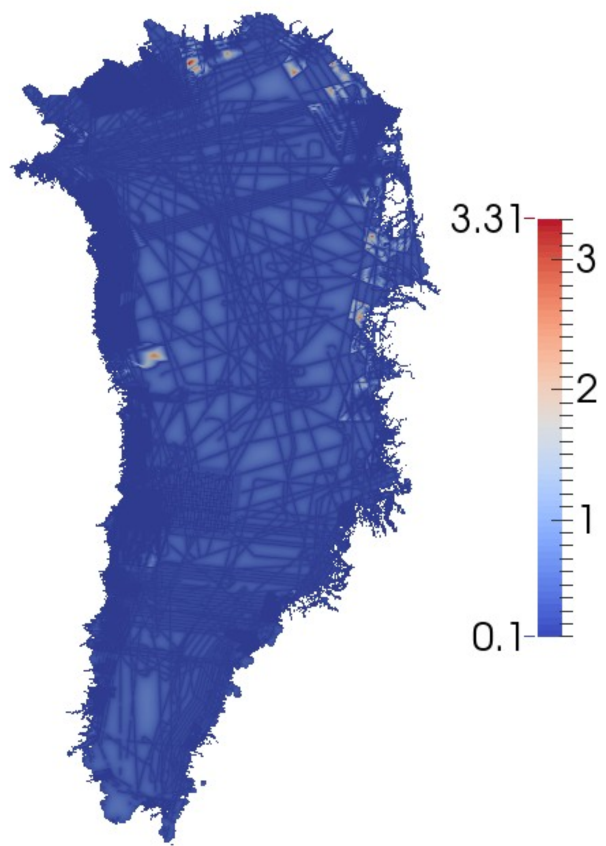
Deterministic Inversion for Greenland ice sheet

Errors associated with velocity and thickness observations

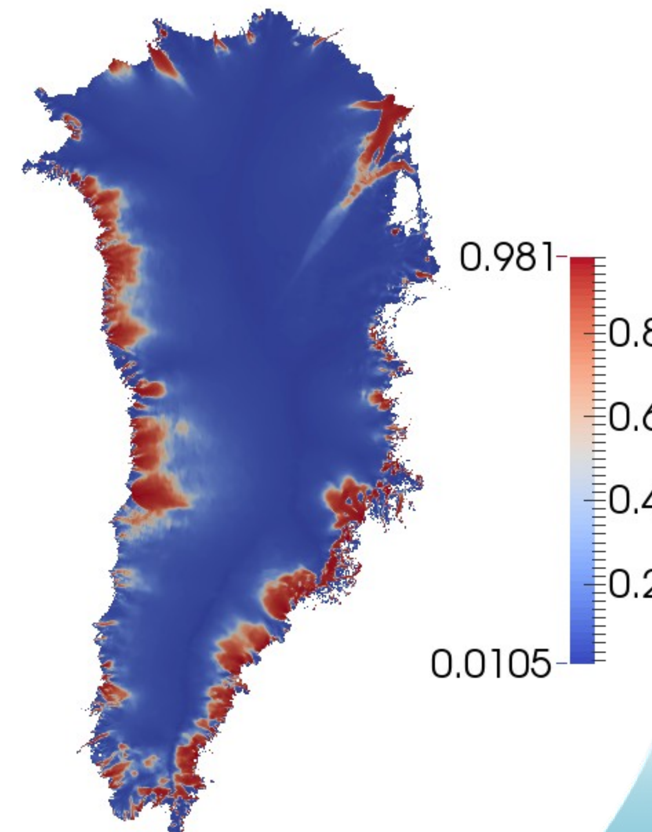
$\sigma_{\mathbf{u}}$: surf. velocity err. in m/yr



σ_H: thickness err. in km



σ_τ: $\dfrac{dH}{dt}$ err. in m/yr

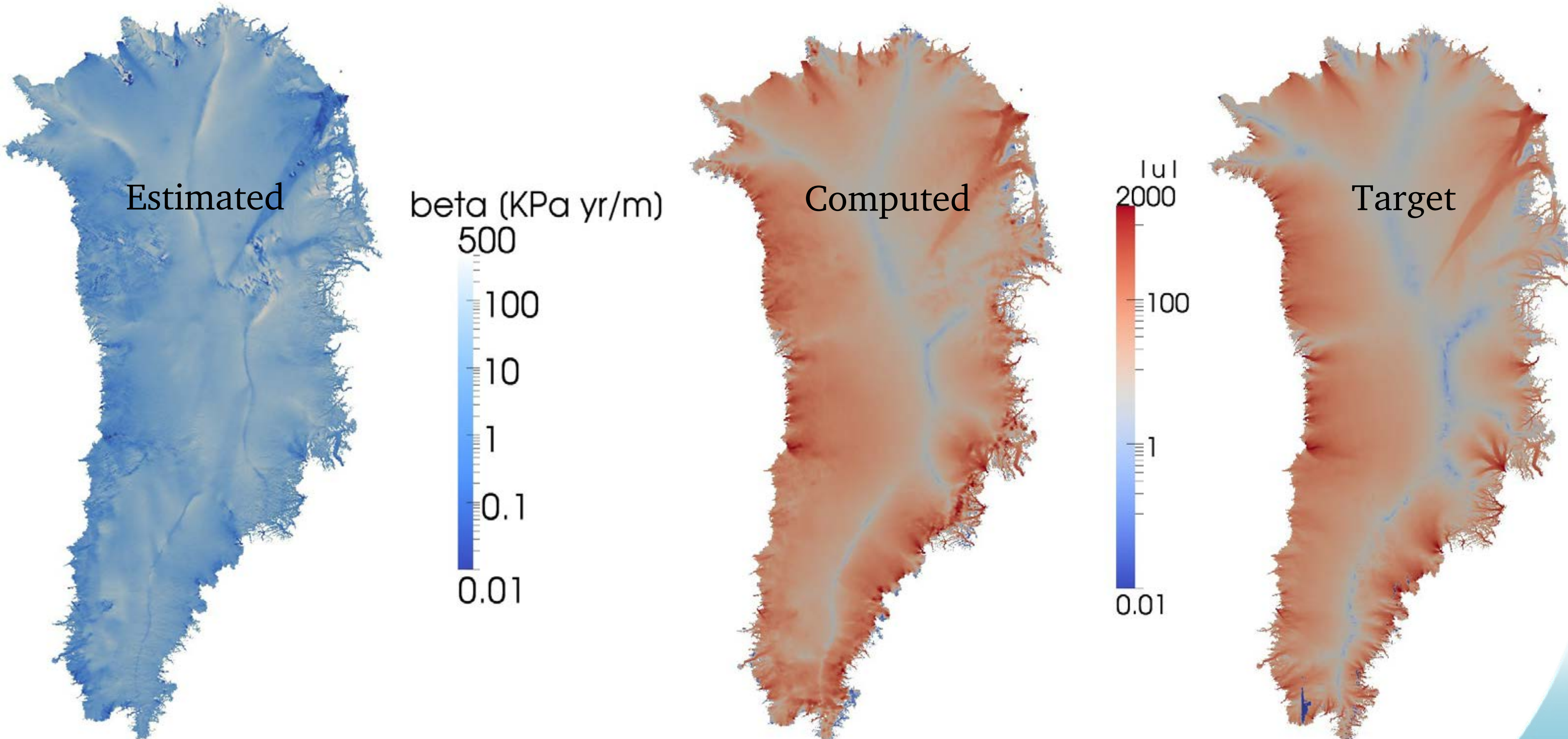


Morlighem et al., Nature Geo., 2014
Error on dH/dt freely based on estimates in *Csatho et. al*, PNAS, 2015.

Greenland Inversion

velocity mismatch only, tuning basal friction

Inversion with 1.6M parameters



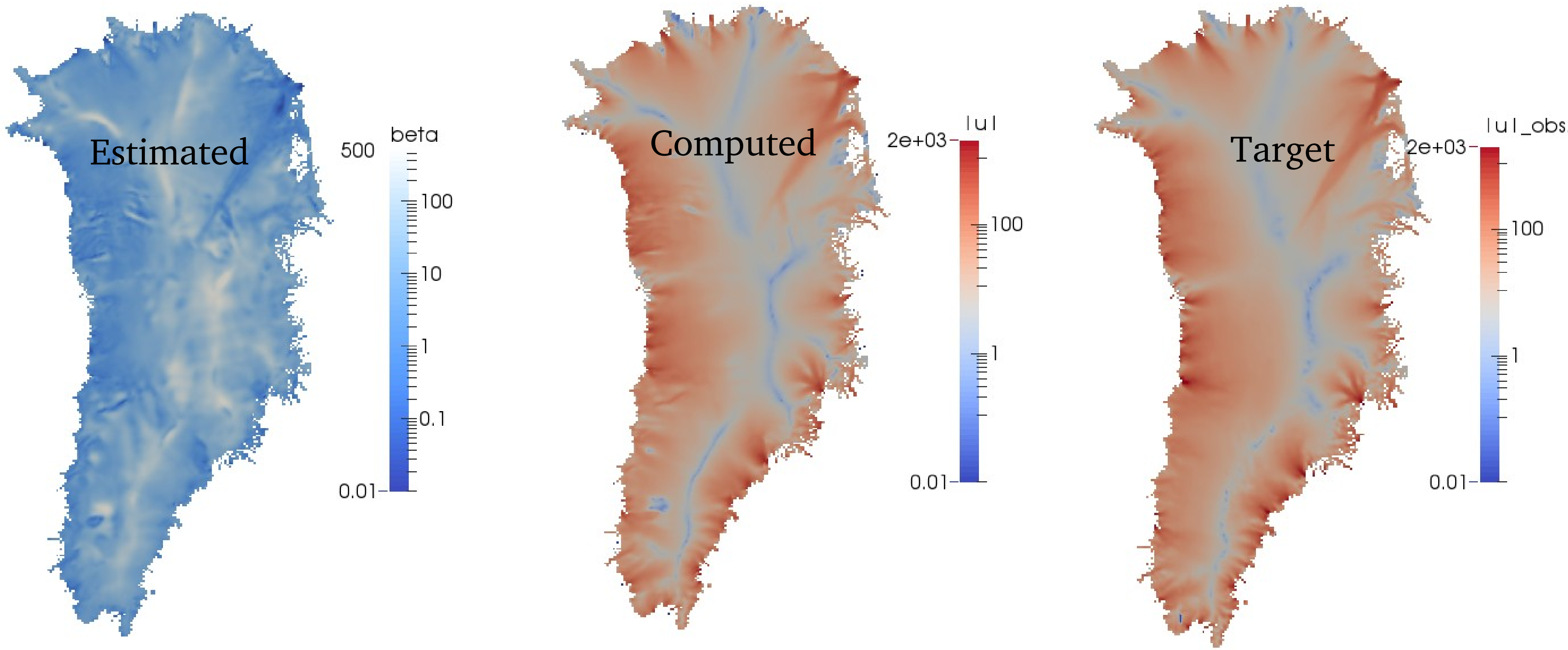
Basal friction coefficient (m/yr)

surface velocity magnitude (m/yr)

Geometry (Morlighem et al., Nature Geo., 2014)

Greenland Inversion

Full inversion



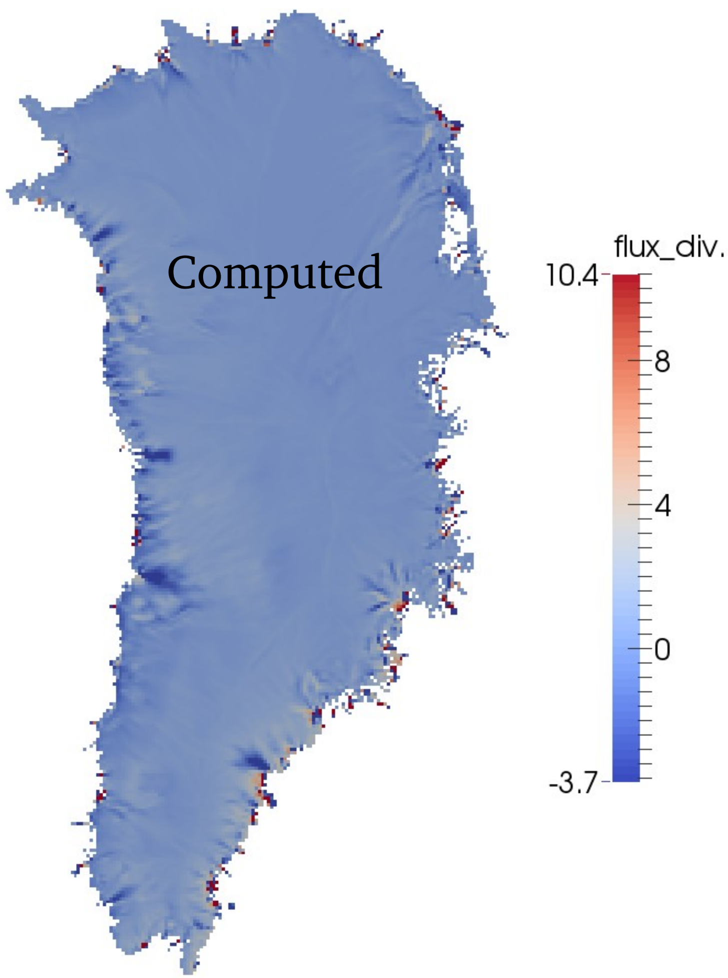
Basal friction coefficient (m/yr)

surface velocity magnitude (m/yr)

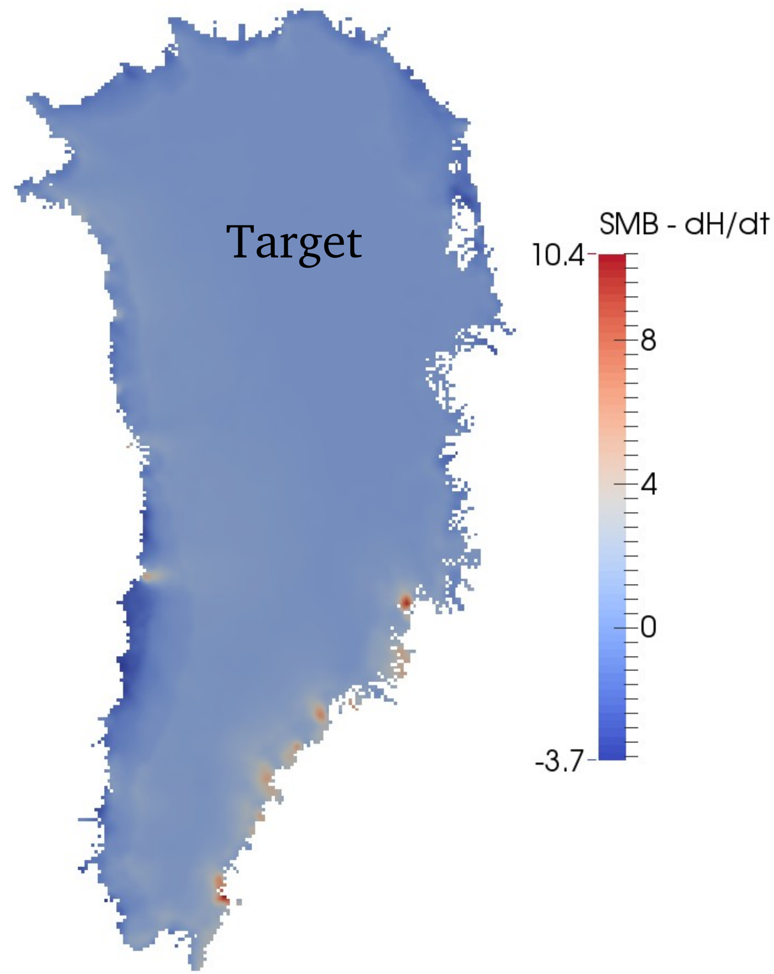
Geometry (Morlighem et al., Nature Geo., 2014)

Greenland Inversion

mismatch with climate forcing



Flux Divergence (m/yr)

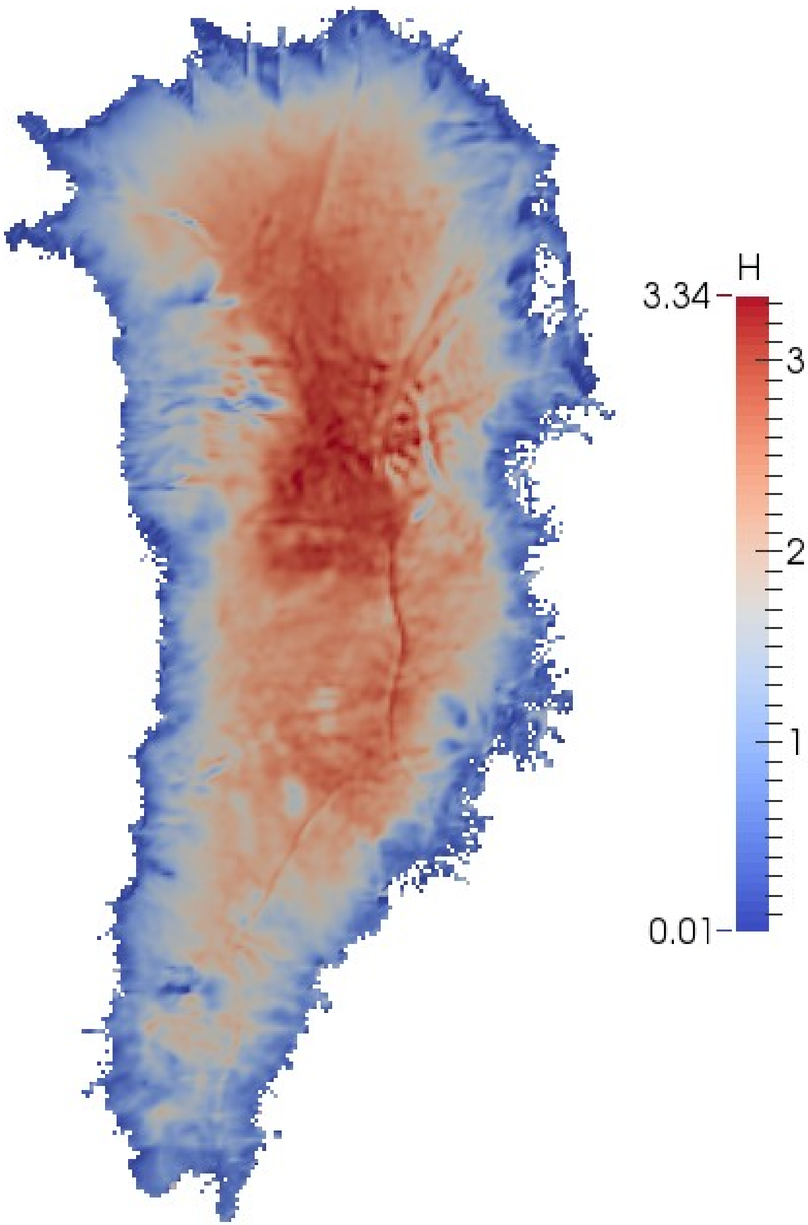


SMB – dH/dt (m/yr)

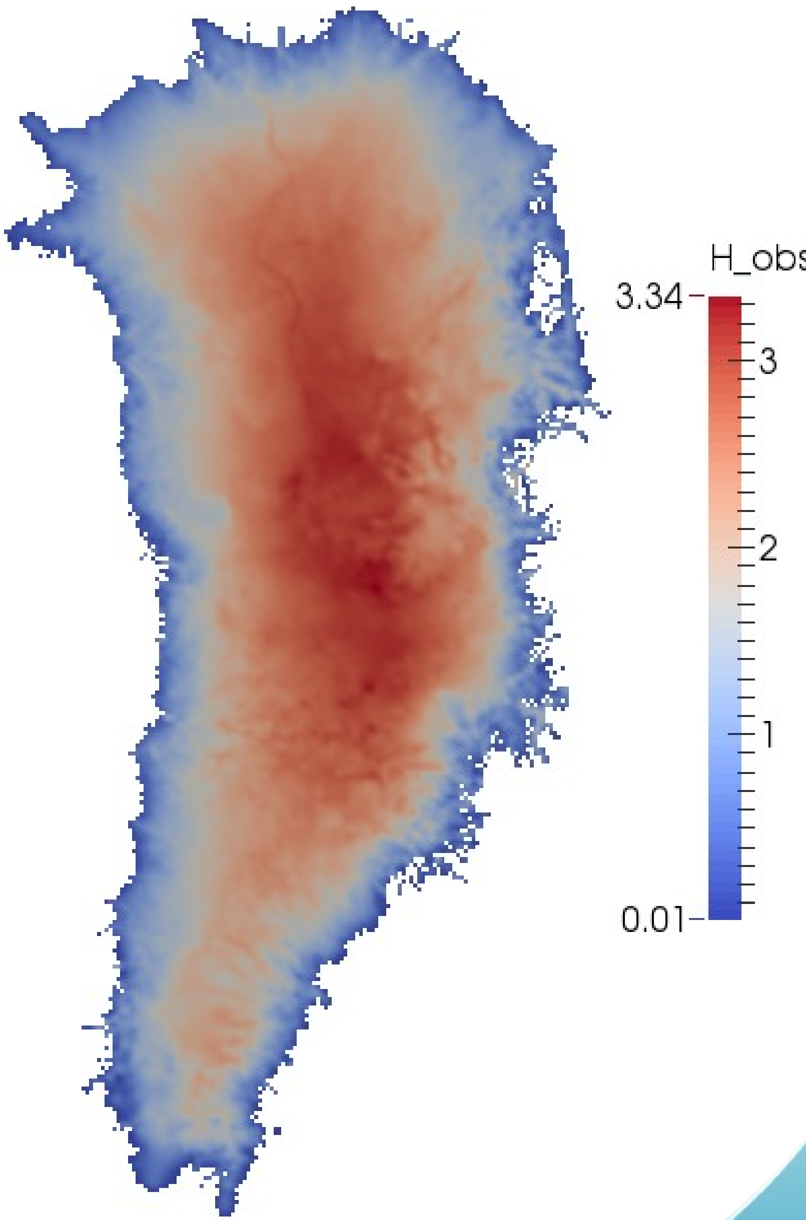
Geometry (Morlighem et al., Nature Geo., 2014)

Greenland Inversion

mismatch with climate forcing



Thickness (km)



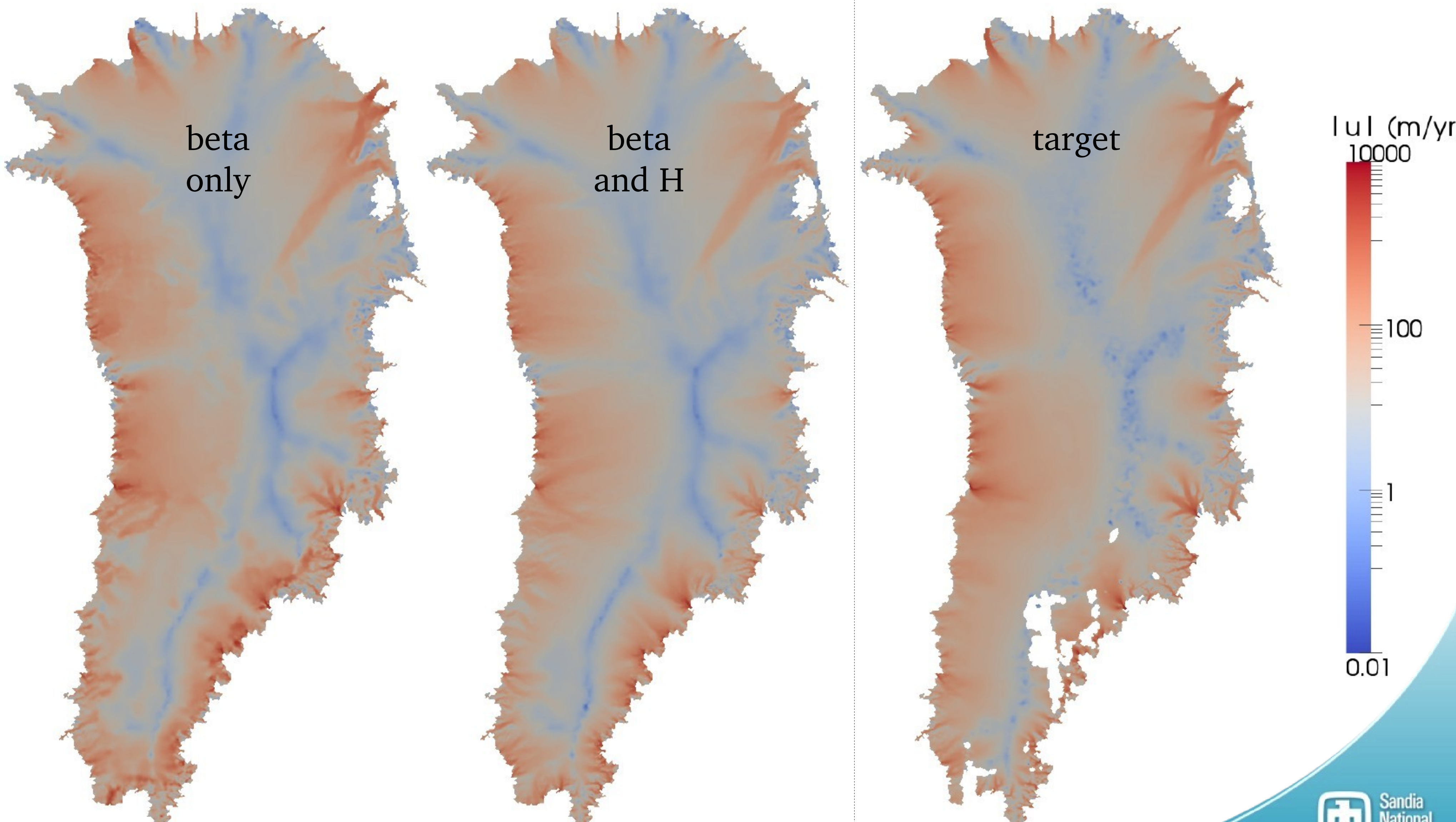
Observed Thickness (km)

Geometry (Morlighem et al., Nature Geo., 2014)

Deterministic Inversion for Greenland ice sheet

Inversion results: surface velocities

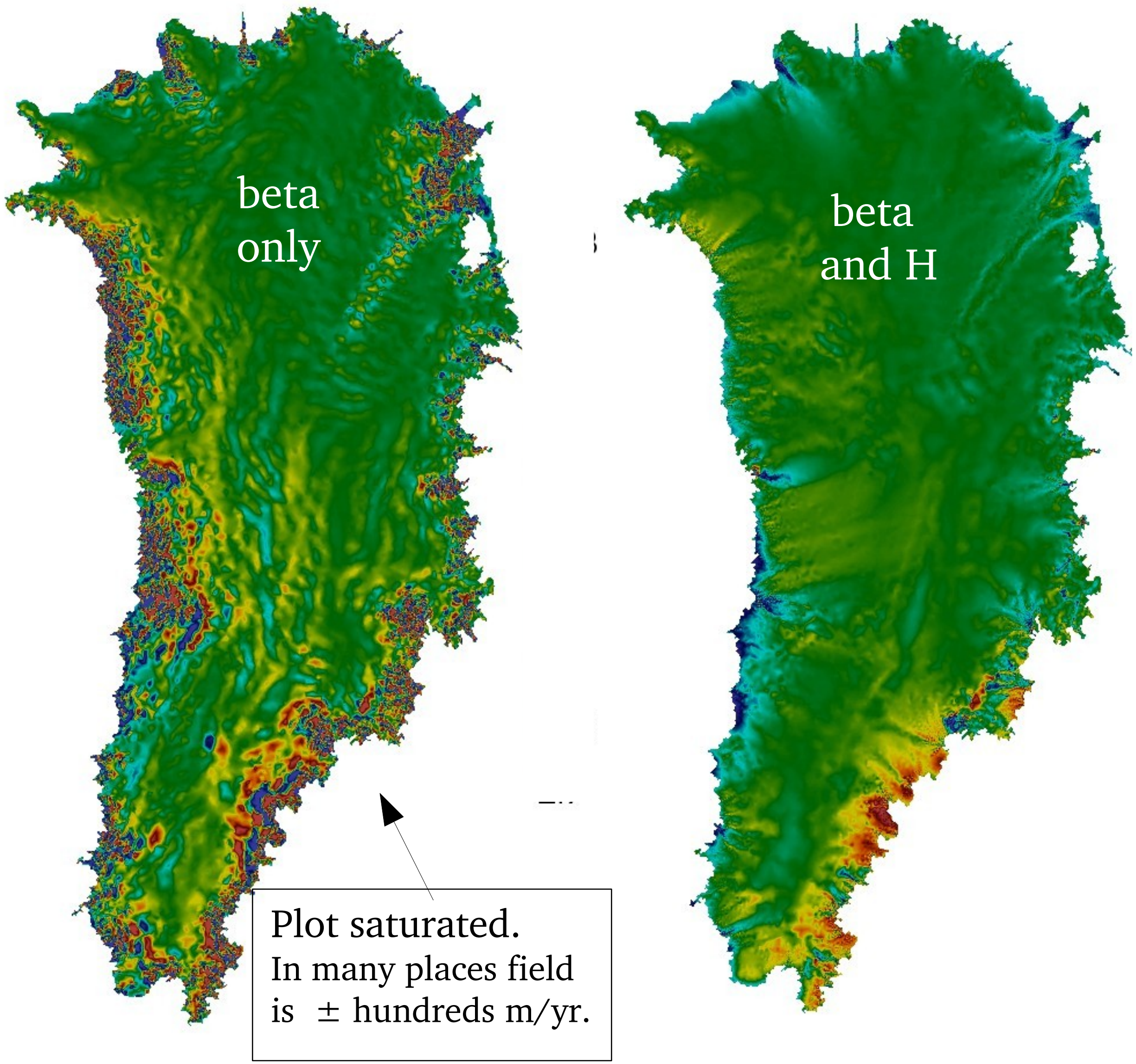
computed surface velocity | observed surface velocity



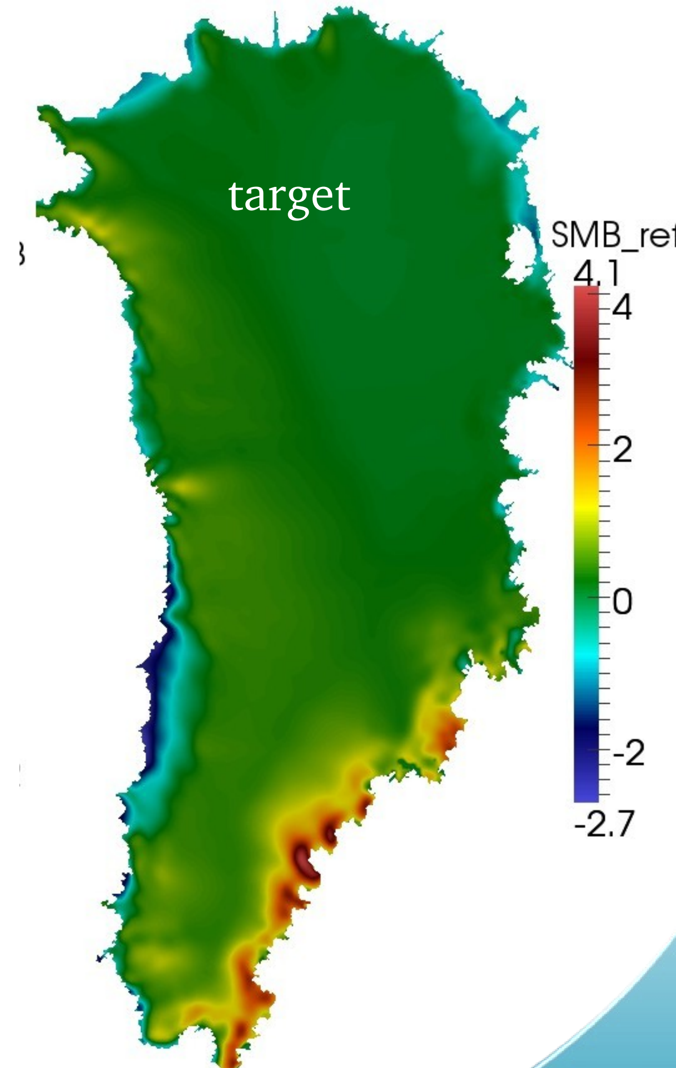
Deterministic Inversion for Greenland ice sheet

Inversion results: surface mass balance (SMB)

SMB (m/yr) needed for equilibrium



SMB from climate model
(Ettema et al. 2009, RACMO2/GR)



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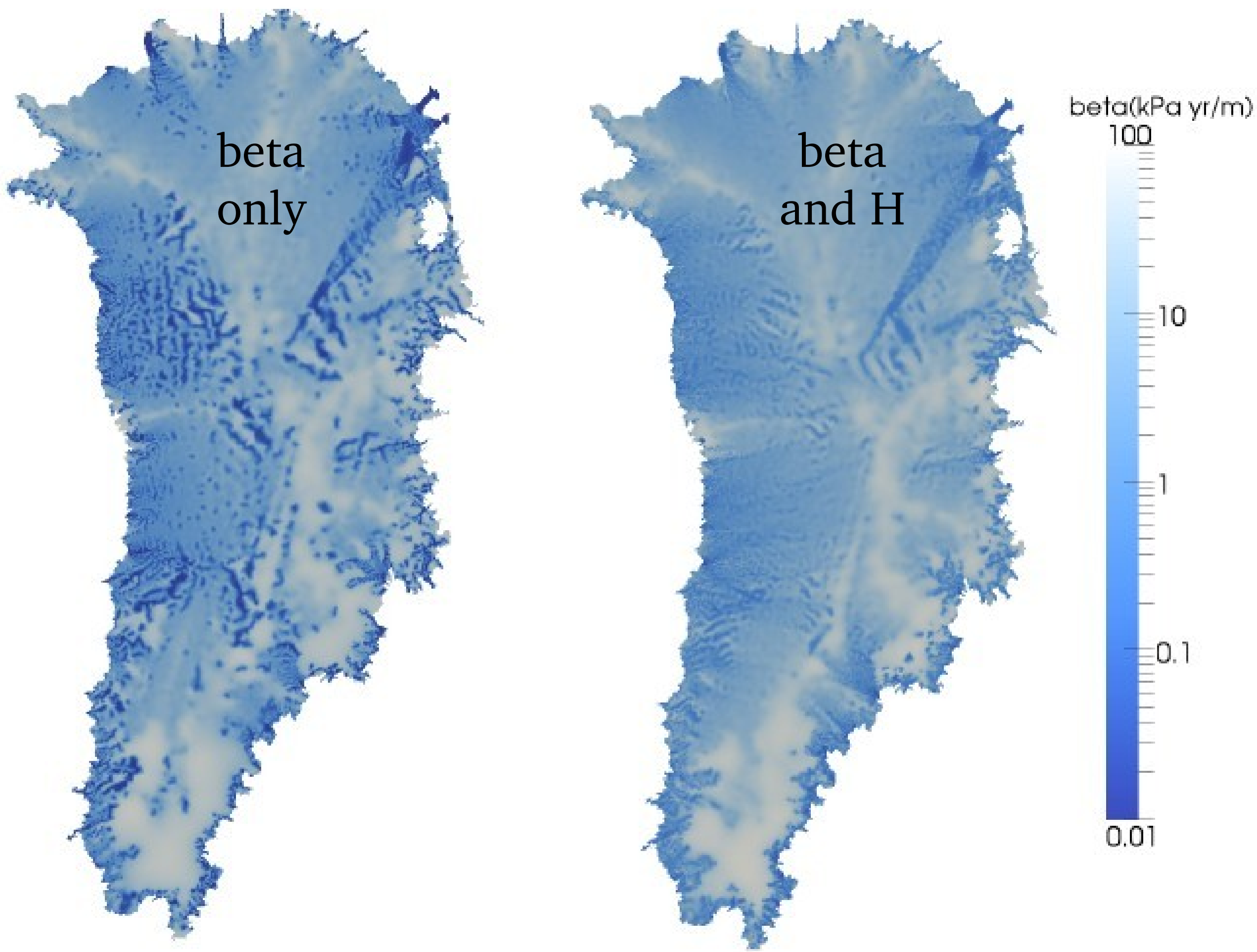
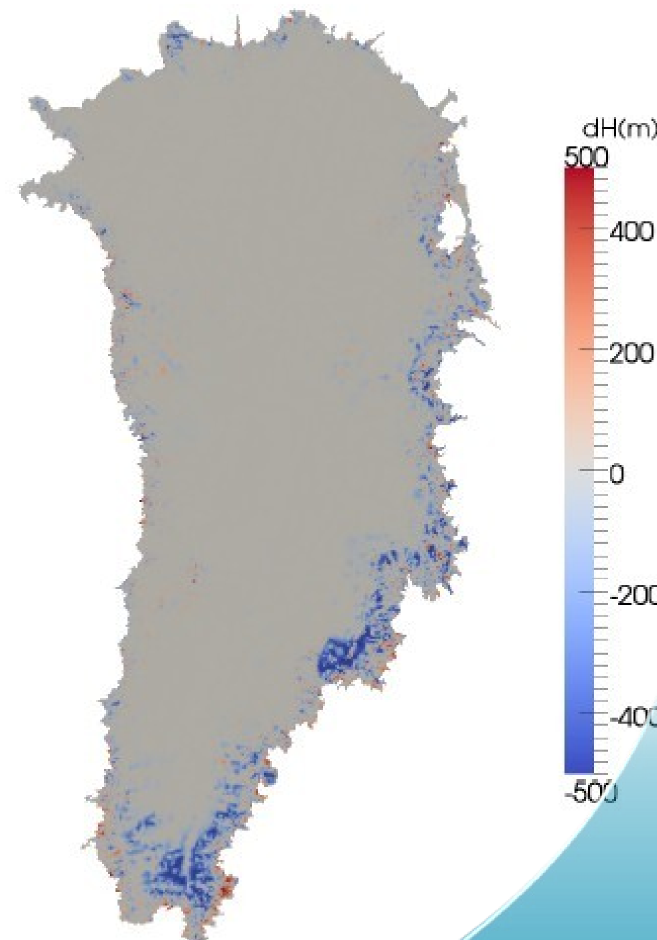
Deterministic Inversion for Greenland ice sheet

Estimated beta and change in topography

recovered basal friction



difference between recovered and observed thickness



Geometry (Morlighem et al., Nature Geo., 2014)

Discussion on inversion

Optimization helps finding an initial state that is somewhat in compliance with observed velocities and with observed climate forcing and ice transients.

The mismatch found is larger then ideal (computed quantities on average 3-4 sigmas away from observations). Possible causes are:

- Temperature is assumed as given, with no uncertainty associated with it.
- Observations of velocity, surface mass balance, bedrock topography do not come from the same dataset and hence effective uncertainty might be bigger than the one provided with the measurement.
- Consider other source of uncertainty, e.g. model parameters (e.g. Glen's law exponent) or the model itself.

Another limit of the current inversion is that the basal friction law does not account for variation in time of the basal friction due to subglacial hydrology*.

*See talk by L. Bertagna in MS32, Wed, 9:35am